



## wwPDB EM Validation Summary Report ⓘ

Jun 18, 2022 – 09:51 am BST

PDB ID : 7PO1  
EMDB ID : EMD-13559  
Title : Initiation complex of human mitochondrial ribosome small subunit with IF3  
Authors : Itoh, Y.; Khawaja, A.; Rorbach, J.; Amunts, A.  
Deposited on : 2021-09-08  
Resolution : 2.92 Å(reported)  
Based on initial model : 6RW4

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev8  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.28.1

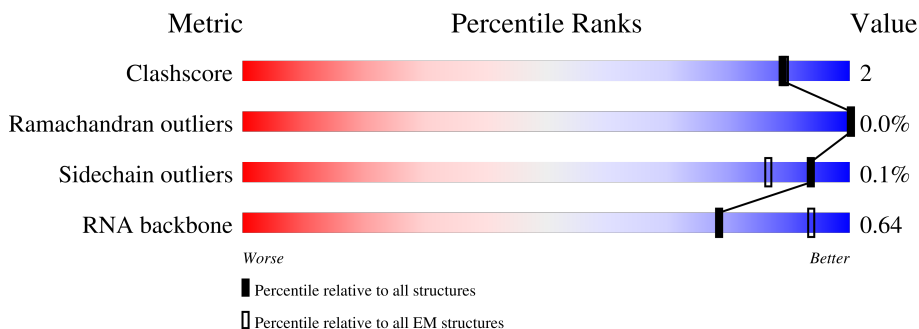
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.92 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	955	
2	B	296	
3	C	167	
4	D	430	
5	E	125	
6	F	242	
7	G	396	

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Mol	Chain	Length	Quality of chain
8	H	201	
9	I	194	
10	J	138	
11	K	128	
12	L	257	
13	M	137	
14	N	130	
15	O	258	
16	P	142	
17	Q	86	
18	R	360	
19	S	190	
20	T	173	
21	U	205	
22	V	414	
23	W	187	
24	X	398	
25	Y	395	
26	Z	106	
27	0	218	
28	1	323	
29	2	117	
30	3	199	
31	4	689	
32	8	278	

## 2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 129179 atoms, of which 59303 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 12S mitochondrial rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	955	Total	C	H	N	O	P	0	0
			30595	9098	10313	3652	6577	955		

- Molecule 2 is a protein called 28S ribosomal protein S2, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	225	Total	C	H	N	O	S	0	0
			3644	1164	1816	331	323	10		

- Molecule 3 is a protein called 28S ribosomal protein S24, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	132	Total	C	H	N	O	S	0	0
			2172	699	1089	195	185	4		

- Molecule 4 is a protein called 28S ribosomal protein S5, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D	343	Total	C	H	N	O	S	0	0
			5536	1713	2805	518	487	13		

- Molecule 5 is a protein called 28S ribosomal protein S6, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	E	122	Total	C	H	N	O	S	0	0
			1973	614	1001	177	177	4		

- Molecule 6 is a protein called 28S ribosomal protein S7, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	F	208	Total	C	H	N	O	S	0	0
			3495	1104	1770	312	298	11		

- Molecule 7 is a protein called 28S ribosomal protein S9, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	G	325	Total	C	H	N	O	S	0	0
			5348	1698	2676	475	485	14		

- Molecule 8 is a protein called 28S ribosomal protein S10, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	H	140	Total	C	H	N	O	S	0	0
			2336	745	1184	194	210	3		

- Molecule 9 is a protein called 28S ribosomal protein S11, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	I	137	Total	C	H	N	O	S	0	0
			2081	642	1061	192	182	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	184	5F0	ASN	conflict	UNP P82912

- Molecule 10 is a protein called 28S ribosomal protein S12, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	J	108	Total	C	H	N	O	S	0	0
			1727	521	888	169	143	6		

- Molecule 11 is a protein called 28S ribosomal protein S14, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	K	101	Total	C	H	N	O	S	0	0
			1748	537	886	179	141	5		

- Molecule 12 is a protein called 28S ribosomal protein S15, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	L	174	Total	C	H	N	O	S	0	0
			2994	925	1541	270	251	7		

- Molecule 13 is a protein called 28S ribosomal protein S16, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	M	119	Total	C	H	N	O	S	0	0
			1908	594	966	185	157	6		

- Molecule 14 is a protein called 28S ribosomal protein S17, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	N	110	Total	C	H	N	O	S	0	0
			1797	562	929	156	147	3		

- Molecule 15 is a protein called 28S ribosomal protein S18b, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	O	193	Total	C	H	N	O	S	0	0
			3149	1014	1557	294	277	7		

- Molecule 16 is a protein called 28S ribosomal protein S18c, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	P	97	Total	C	H	N	O	S	0	0
			1588	501	807	134	138	8		

- Molecule 17 is a protein called 28S ribosomal protein S21, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	Q	86	Total	C	H	N	O	S	0	0
			1502	460	758	150	126	8		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	50	ARG	CYS	variant	UNP P82921

- Molecule 18 is a protein called 28S ribosomal protein S22, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	R	295	Total	C	H	N	O	S	0	0
			4838	1533	2429	413	455	8		

- Molecule 19 is a protein called 28S ribosomal protein S23, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	S	135	Total	C	H	N	O	S	0	0
			2227	716	1116	198	196	1		

- Molecule 20 is a protein called 28S ribosomal protein S25, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	T	168	Total	C	H	N	O	S	0	0
			2765	877	1394	239	244	11		

- Molecule 21 is a protein called 28S ribosomal protein S26, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	U	176	Total	C	H	N	O	S	0	0
			2988	916	1500	301	267	4		

- Molecule 22 is a protein called 28S ribosomal protein S27, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	V	362	Total	C	H	N	O	S	0	0
			5933	1904	2964	495	558	12		

- Molecule 23 is a protein called 28S ribosomal protein S28, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	W	100	Total	C	H	N	O	S	0	0
			1592	498	803	141	146	4		

- Molecule 24 is a protein called 28S ribosomal protein S29, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	X	352	Total	C	H	N	O	S	0	0
			5694	1822	2845	499	517	11		

- Molecule 25 is a protein called 28S ribosomal protein S31, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	Y	149	Total	C	H	N	O	S	0	0
			2444	801	1198	207	234	4		

- Molecule 26 is a protein called 28S ribosomal protein S33, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	Z	100	Total	C	H	N	O	S	0	0
			1699	534	860	153	148	4		

- Molecule 27 is a protein called 28S ribosomal protein S34, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	0	215	Total	C	H	N	O	S	0	0
			3584	1130	1797	339	313	5		

- Molecule 28 is a protein called 28S ribosomal protein S35, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	1	276	Total	C	H	N	O	S	0	0
			4507	1419	2269	381	427	11		

- Molecule 29 is a protein called Coiled-coil-helix-coiled-coil-helix domain-containing protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	2	117	Total	C	H	N	O	S	0	0
			1904	579	969	182	166	8		

- Molecule 30 is a protein called Aurora kinase A-interacting protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
30	3	71	Total	C	H	N	O	S	0	0
			1331	403	702	135	90	1		

- Molecule 31 is a protein called Pentatricopeptide repeat domain-containing protein 3, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	4	592	Total	C	H	N	O	S	0	0
			9593	3070	4798	812	885	28		

- Molecule 32 is a protein called Mitochondrial translational initiation factor 3, isoform CRA\_a.

Mol	Chain	Residues	Atoms						AltConf	Trace
32	8	191	Total	C	H	N	O	S	0	0
			3131	953	1588	289	293	8		

There is a discrepancy between the modelled and reference sequences:



Chain	Residue	Modelled	Actual	Comment	Reference
8	68	ILE	THR	variant	UNP A0A024RDQ7

- Molecule 33 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
33	A	68	Total 68	Mg 68	0
33	B	1	Total 1	Mg 1	0
33	X	1	Total 1	Mg 1	0
33	3	1	Total 1	Mg 1	0

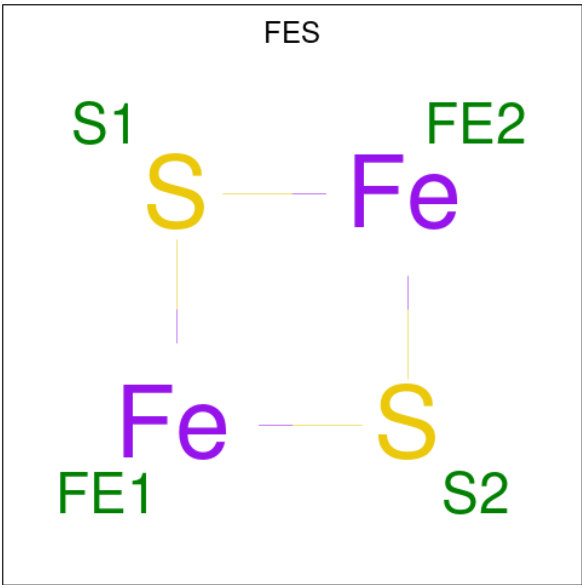
- Molecule 34 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
34	A	20	Total 20	K 20	0

- Molecule 35 is ZINC ION (three-letter code: ZN) (formula: Zn).

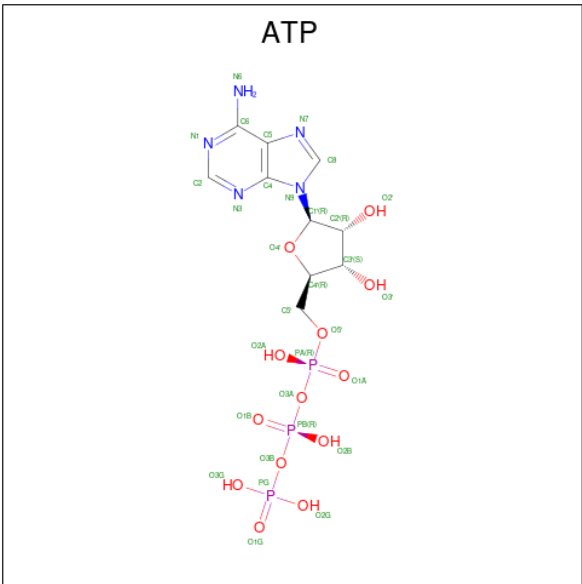
Mol	Chain	Residues	Atoms		AltConf
35	O	1	Total 1	Zn 1	0

- Molecule 36 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



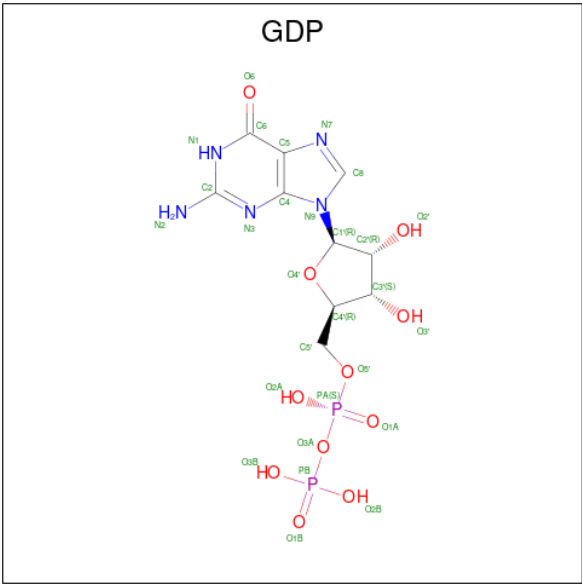
Mol	Chain	Residues	Atoms			AltConf
36	P	1	Total	Fe	S	0
			4	2	2	
36	T	1	Total	Fe	S	0
			4	2	2	

- Molecule 37 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms						AltConf
37	X	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

- Molecule 38 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>11</sub>P<sub>2</sub>).



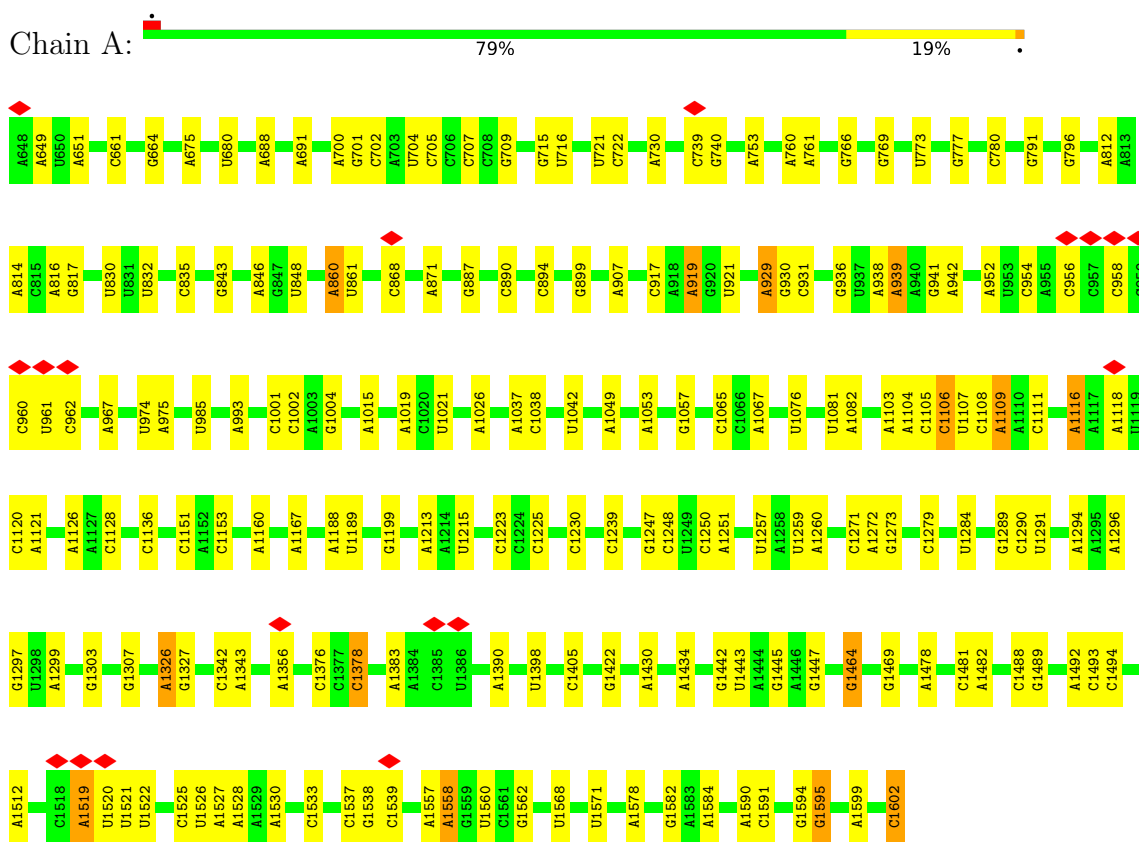
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Mol	Chain	Residues	Atoms		AltConf
39	J	6	Total 6	O 6	0
39	K	27	Total 27	O 27	0
39	L	7	Total 7	O 7	0
39	M	23	Total 23	O 23	0
39	N	10	Total 10	O 10	0
39	O	16	Total 16	O 16	0
39	P	11	Total 11	O 11	0
39	Q	15	Total 15	O 15	0
39	R	8	Total 8	O 8	0
39	S	11	Total 11	O 11	0
39	T	9	Total 9	O 9	0
39	U	3	Total 3	O 3	0
39	W	8	Total 8	O 8	0
39	X	5	Total 5	O 5	0
39	Y	5	Total 5	O 5	0
39	Z	14	Total 14	O 14	0
39	0	18	Total 18	O 18	0
39	1	14	Total 14	O 14	0
39	2	10	Total 10	O 10	0
39	3	11	Total 11	O 11	0
39	4	3	Total 3	O 3	0

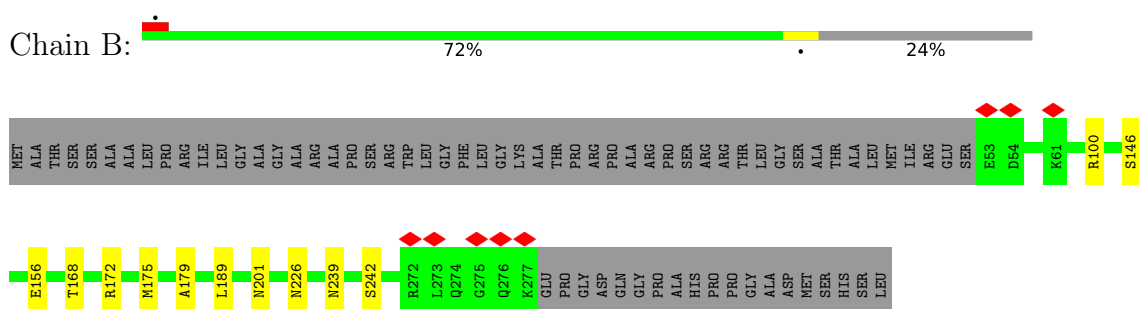
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: 12S mitochondrial rRNA

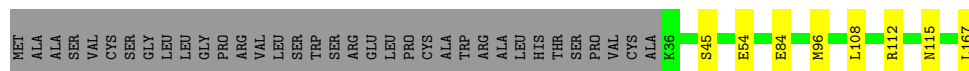


#### • Molecule 2: 28S ribosomal protein S2, mitochondrial




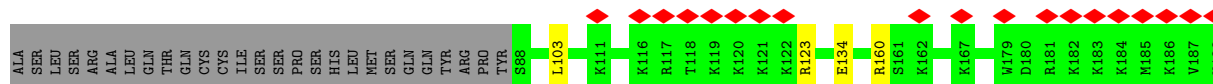
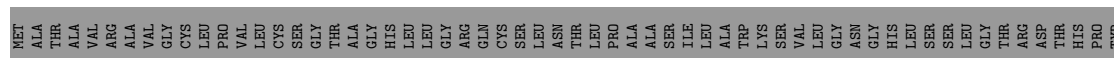
- Molecule 3: 28S ribosomal protein S24, mitochondrial

Chain C:  74% 5% 21%



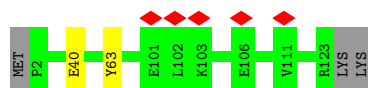
- Molecule 4: 28S ribosomal protein S5, mitochondrial

Chain D:  5% 77% 20%




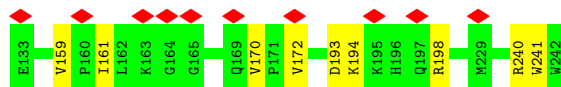
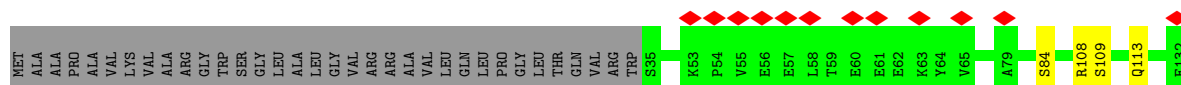
- Molecule 5: 28S ribosomal protein S6, mitochondrial

Chain E:  96% 4% 0%




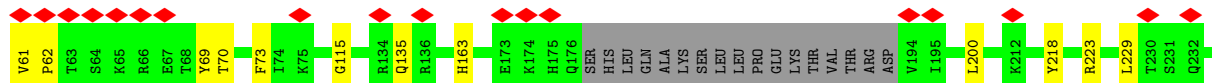
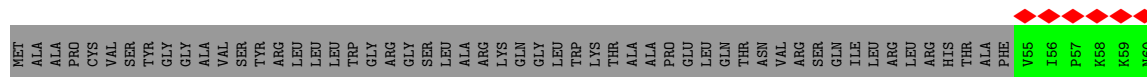
- Molecule 6: 28S ribosomal protein S7, mitochondrial

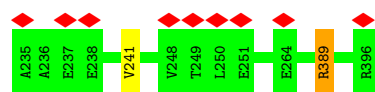
Chain F:  9% 81% 5% 14%



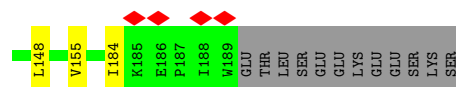
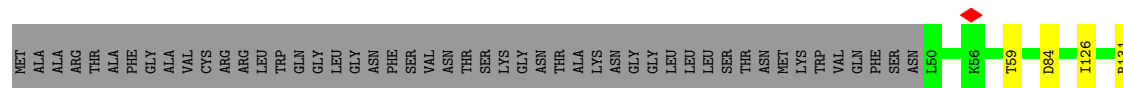
- Molecule 7: 28S ribosomal protein S9, mitochondrial

Chain G:  8% 79% 13% 0%

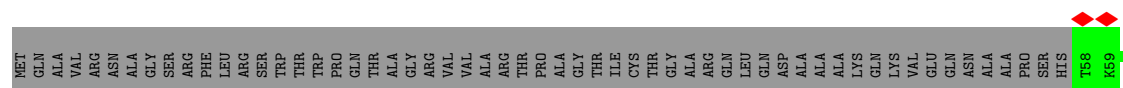




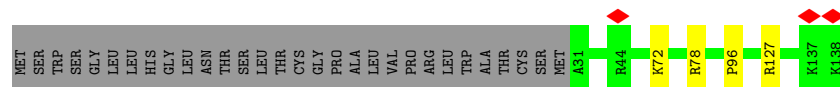
- Molecule 8: 28S ribosomal protein S10, mitochondrial



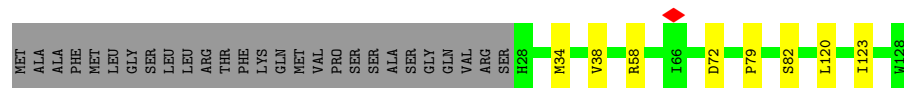
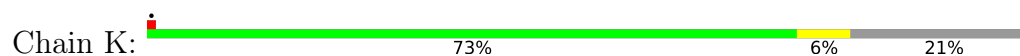
- Molecule 9: 28S ribosomal protein S11, mitochondrial



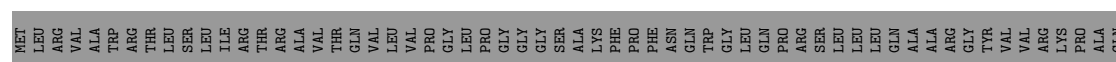
- Molecule 10: 28S ribosomal protein S12, mitochondrial

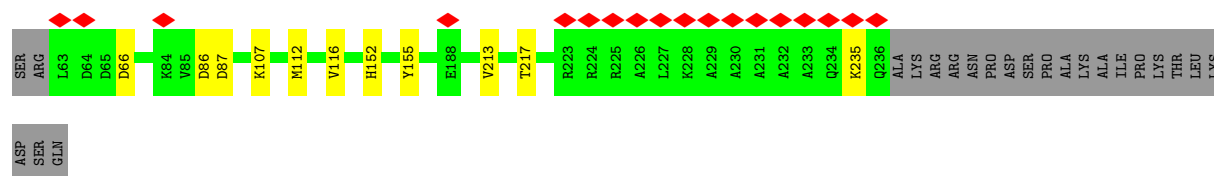


- Molecule 11: 28S ribosomal protein S14, mitochondrial

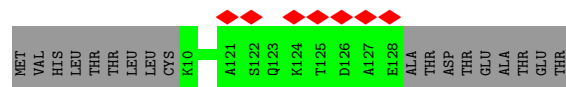
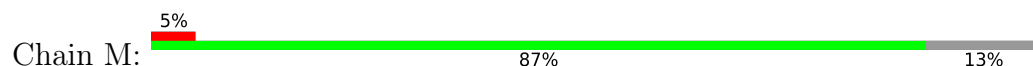


- Molecule 12: 28S ribosomal protein S15, mitochondrial

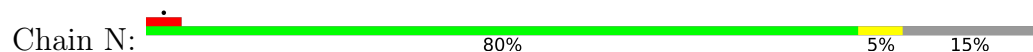




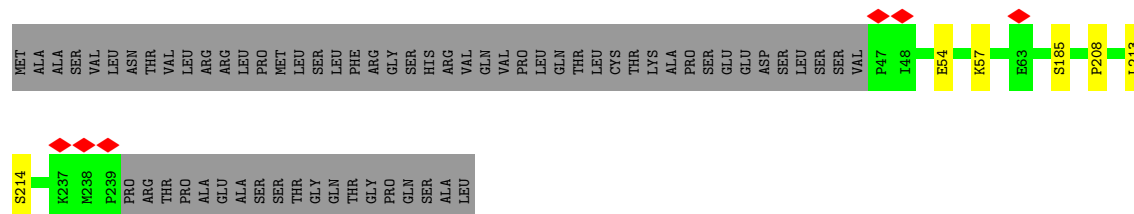
- Molecule 13: 28S ribosomal protein S16, mitochondrial



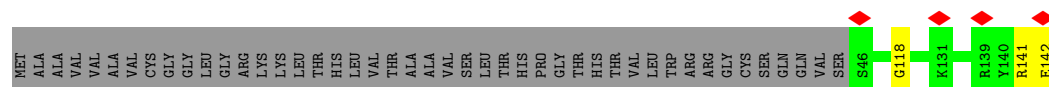
- Molecule 14: 28S ribosomal protein S17, mitochondrial



- Molecule 15: 28S ribosomal protein S18b, mitochondrial



- Molecule 16: 28S ribosomal protein S18c, mitochondrial

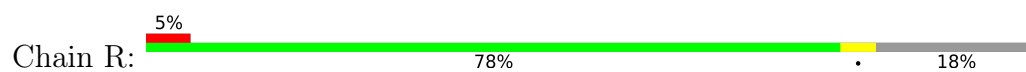


- Molecule 17: 28S ribosomal protein S21, mitochondrial



- Molecule 18: 28S ribosomal protein S22, mitochondrial





MET ALA SER PRO LEU THR THR VAL LEU LEU TRP SER SER LEU ARG SER SER PRO GLY VAL ARG ARG CYS PHE ARG ALA ARG ILE GLN PRO TRP HIS GLY GLY LEU LEU GLN PRO LEU PRO CYS SER PHE MET GLY LEU PRO ARG ARG ARG PHE SER SER SER ALA ALA ALA GLU SER

GLY SER E84 T65 K66 K67 L142 I161 S162 H167 R170 K183 I193 Y219 D238 R256 L262 T265 V276 Q302 V306 L307 A317 K319 D319 Q320 E323 K329 K338 E343 A352 L353 S354 R355 H356 S357 A358 SER

- Molecule 19: 28S ribosomal protein S23, mitochondrial



MET A2 V51 Q82 K93 C96 V100 E101 K102 L106 Q107 K108 L109 G110 E111 T112 D113 E114 E115 K116 L117 K123 A124 L125 L126 A127 E128 G129 V130 I131 L132 R133 R134 V135 G136 GLU ALA THR GLN HIS GLY GLY SER HIS VAL SER ARG LYS SER GLU HIS LEU

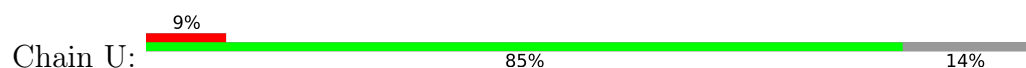
SER VAL ARG PRO GLN THR ALA LEU GLU ASN THR GLN LYS VAL PRO GLN ASP GLN HIS LEU GLU ALA PRO ALA ASP GLN LYS GLY A124 L125 LEU PRO PRO

- Molecule 20: 28S ribosomal protein S25, mitochondrial



MET P2 V32 L76 T92 E110 R114 E115 K120 K121 H125 R132 L136 A165 A166 L167 K168 A169 ASP ALA GLN ASP

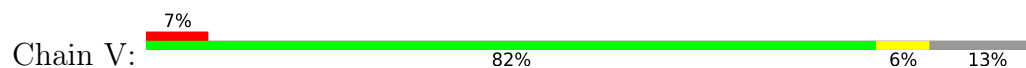
- Molecule 21: 28S ribosomal protein S26, mitochondrial



MET LEU ARG ALA LEU SER ARG LEU GLY ALA GLY THR PRO CYS ARG PRO ARG ALA LEU VAL LEU PRO PRO ARG GLY R27 K36 E40 V89 R93 L96 R129 E130 Q131 E132 Q135 E138 Q139 A140 R141 K142 A143 E144 E145 V146 Q147 Y167 Q201 R202

ARG ASP SER

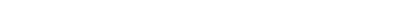
- Molecule 22: 28S ribosomal protein S27, mitochondrial

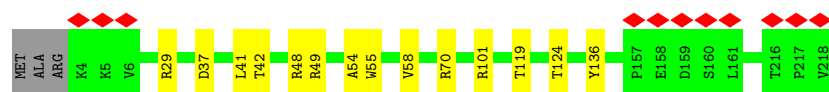


MET ALA ALA SER ILE VAL ARG ARG GLY MET LEU LEU ALA ARG GLN VAL VAL PRO GLN LEU SER PRO PRO GLY ALA LYS TYR L29 L30 V35 K39 C49 L50 E62 R63 L129 N141 F144 D149 A172 L190 A191 K192 K193 T194 L208 K216

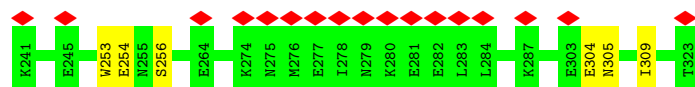
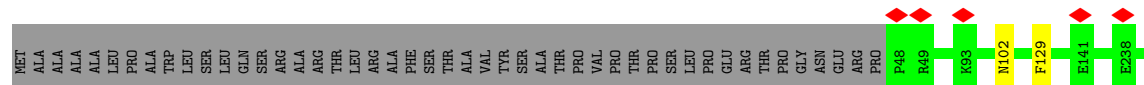
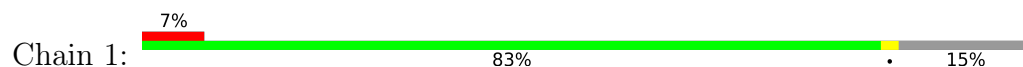
L225 Y226 L236 E271 L275 L280 L283 L290 T291 S292 A293 ASP GLY ALA SER SER SER GLU GLU GLN SER GLN ASN ASP GLU ASN ASN GLN SER E311 K312 L319 E323 K335 K340 A343 L344 E348 V360 K361 L364 E376 E398 Q399

A400 K401 Q402 E403 Y404 Q405 A406 Q407 LYS ALA ALA LYS ALA SER SER ALA

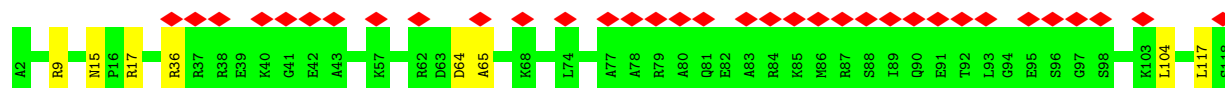
- Chain 0:  5% 92% 6%



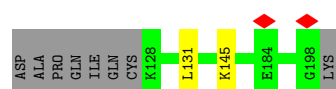
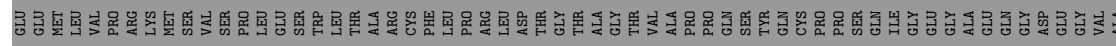
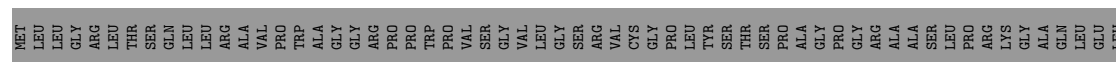
- Molecule 28: 28S ribosomal protein S35, mitochondrial



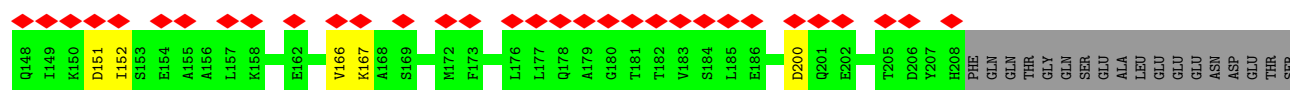
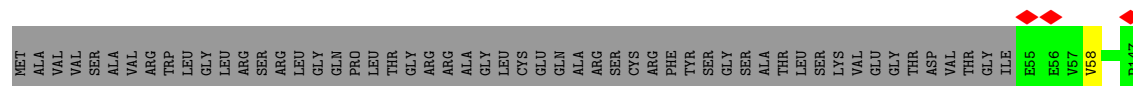
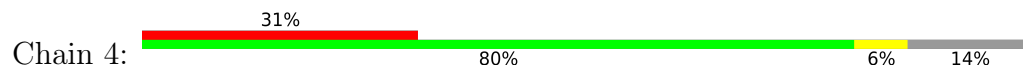
- Molecule 29: Coiled-coil-helix-coiled-coil-helix domain-containing protein 1

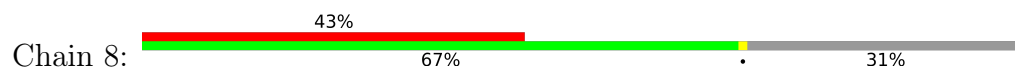


- Molecule 30: Aurora kinase A-interacting protein



- Molecule 31: Pentatricopeptide repeat domain-containing protein 3, mitochondrial





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	45435	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	31	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	165000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.797	Depositor
Minimum map value	-0.770	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.033	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	388.8, 388.8, 388.8	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.648, 0.648, 0.648	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: K, AYA, 5F0, MG, GDP, 5MU, ZN, B8T, 5MC, FES, ATP, MA6

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.26	0/22562	0.67	0/35124
2	B	0.25	0/1871	0.41	0/2531
3	C	0.26	0/1113	0.41	0/1505
4	D	0.25	0/2783	0.42	0/3724
5	E	0.25	0/989	0.42	0/1335
6	F	0.24	0/1767	0.36	0/2373
7	G	0.25	0/2729	0.39	0/3658
8	H	0.25	0/1178	0.42	0/1598
9	I	0.26	0/1030	0.43	0/1386
10	J	0.26	0/855	0.46	0/1148
11	K	0.23	0/880	0.41	0/1182
12	L	0.24	0/1477	0.36	0/1974
13	M	0.25	0/963	0.42	0/1295
14	N	0.25	0/886	0.45	0/1199
15	O	0.25	0/1648	0.40	0/2243
16	P	0.26	0/798	0.41	0/1070
17	Q	0.24	0/748	0.39	0/994
18	R	0.25	0/2456	0.38	0/3317
19	S	0.26	0/1138	0.39	0/1533
20	T	0.25	0/1402	0.40	0/1883
21	U	0.23	0/1510	0.37	0/2025
22	V	0.23	0/3030	0.35	0/4093
23	W	0.26	0/801	0.42	0/1079
24	X	0.24	0/2921	0.38	0/3954
25	Y	0.24	0/1280	0.37	0/1725
26	Z	0.25	0/857	0.39	0/1141
27	0	0.25	0/1834	0.41	0/2484
28	1	0.24	0/2285	0.38	0/3090
29	2	0.23	0/941	0.38	0/1257
30	3	0.24	0/640	0.38	0/844
31	4	0.24	0/4904	0.36	0/6636
32	8	0.23	0/1560	0.39	0/2089

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
All	All	0.25	0/71836	0.51	0/101489

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	20282	10313	10297	67	0
2	B	1828	1816	1815	8	0
3	C	1083	1089	1088	6	0
4	D	2731	2805	2804	9	0
5	E	972	1001	1000	2	0
6	F	1725	1770	1769	12	0
7	G	2672	2676	2673	9	0
8	H	1152	1184	1183	8	0
9	I	1020	1061	1052	5	0
10	J	839	888	887	3	0
11	K	862	886	885	4	0
12	L	1453	1541	1540	7	0
13	M	942	966	965	0	0
14	N	868	929	928	4	0
15	O	1592	1557	1557	4	0
16	P	781	807	806	2	0
17	Q	744	758	758	5	0
18	R	2409	2429	2428	10	0
19	S	1111	1116	1115	4	0
20	T	1371	1394	1393	4	0
21	U	1488	1500	1499	1	0
22	V	2969	2964	2961	15	0
23	W	789	803	802	0	0
24	X	2849	2845	2843	13	0
25	Y	1246	1198	1197	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	Z	839	860	858	3	0
27	0	1787	1797	1796	10	0
28	1	2238	2269	2269	6	0
29	2	935	969	971	8	0
30	3	629	702	702	2	0
31	4	4795	4798	4796	24	0
32	8	1543	1588	1587	4	0
33	3	1	0	0	0	0
33	A	68	0	0	0	0
33	B	1	0	0	0	0
33	X	1	0	0	0	0
34	A	20	0	0	0	0
35	O	1	0	0	0	0
36	P	4	0	0	0	0
36	T	4	0	0	0	0
37	X	31	12	12	0	0
38	X	28	12	12	0	0
39	0	18	0	0	1	0
39	1	14	0	0	1	0
39	2	10	0	0	0	0
39	3	11	0	0	0	0
39	4	3	0	0	0	0
39	A	762	0	0	12	0
39	B	39	0	0	1	0
39	C	29	0	0	2	0
39	D	29	0	0	0	0
39	E	8	0	0	0	0
39	F	6	0	0	1	0
39	G	29	0	0	1	0
39	H	25	0	0	1	0
39	I	12	0	0	0	0
39	J	6	0	0	0	0
39	K	27	0	0	0	0
39	L	7	0	0	0	0
39	M	23	0	0	0	0
39	N	10	0	0	0	0
39	O	16	0	0	0	0
39	P	11	0	0	0	0
39	Q	15	0	0	0	0
39	R	8	0	0	0	0
39	S	11	0	0	0	0
39	T	9	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	U	3	0	0	0	0
39	W	8	0	0	0	0
39	X	5	0	0	0	0
39	Y	5	0	0	0	0
39	Z	14	0	0	0	0
All	All	69876	59303	59248	216	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

The worst 5 of 216 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1294:A:OP1	2:B:201:ASN:ND2	2.13	0.82
1:A:1342:C:OP2	26:Z:96:LYS:NZ	2.23	0.71
1:A:1021:U:OP2	29:2:9:ARG:NH2	2.23	0.70
15:O:54:GLU:OE1	15:O:57:LYS:NZ	2.24	0.69
22:V:39:LYS:NZ	22:V:376:GLU:OE2	2.25	0.69

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	223/296 (75%)	222 (100%)	1 (0%)	0	100	100
3	C	130/167 (78%)	127 (98%)	3 (2%)	0	100	100
4	D	341/430 (79%)	334 (98%)	7 (2%)	0	100	100
5	E	120/125 (96%)	120 (100%)	0	0	100	100
6	F	206/242 (85%)	204 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	G	321/396 (81%)	316 (98%)	5 (2%)	0	100	100
8	H	138/201 (69%)	136 (99%)	1 (1%)	1 (1%)	22	53
9	I	133/194 (69%)	131 (98%)	2 (2%)	0	100	100
10	J	106/138 (77%)	104 (98%)	2 (2%)	0	100	100
11	K	99/128 (77%)	98 (99%)	1 (1%)	0	100	100
12	L	172/257 (67%)	172 (100%)	0	0	100	100
13	M	117/137 (85%)	117 (100%)	0	0	100	100
14	N	108/130 (83%)	108 (100%)	0	0	100	100
15	O	191/258 (74%)	189 (99%)	2 (1%)	0	100	100
16	P	95/142 (67%)	94 (99%)	1 (1%)	0	100	100
17	Q	84/86 (98%)	84 (100%)	0	0	100	100
18	R	293/360 (81%)	286 (98%)	7 (2%)	0	100	100
19	S	133/190 (70%)	132 (99%)	1 (1%)	0	100	100
20	T	166/173 (96%)	164 (99%)	2 (1%)	0	100	100
21	U	174/205 (85%)	174 (100%)	0	0	100	100
22	V	358/414 (86%)	355 (99%)	3 (1%)	0	100	100
23	W	98/187 (52%)	97 (99%)	1 (1%)	0	100	100
24	X	350/398 (88%)	346 (99%)	4 (1%)	0	100	100
25	Y	147/395 (37%)	146 (99%)	1 (1%)	0	100	100
26	Z	98/106 (92%)	97 (99%)	1 (1%)	0	100	100
27	0	213/218 (98%)	212 (100%)	1 (0%)	0	100	100
28	1	274/323 (85%)	271 (99%)	3 (1%)	0	100	100
29	2	115/117 (98%)	115 (100%)	0	0	100	100
30	3	69/199 (35%)	68 (99%)	1 (1%)	0	100	100
31	4	588/689 (85%)	581 (99%)	7 (1%)	0	100	100
32	8	189/278 (68%)	186 (98%)	3 (2%)	0	100	100
All	All	5849/7579 (77%)	5786 (99%)	62 (1%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	H	126	ILE

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	198/249 (80%)	198 (100%)	0	100	100
3	C	115/143 (80%)	115 (100%)	0	100	100
4	D	286/357 (80%)	286 (100%)	0	100	100
5	E	104/107 (97%)	104 (100%)	0	100	100
6	F	185/209 (88%)	185 (100%)	0	100	100
7	G	284/342 (83%)	283 (100%)	1 (0%)	91	97
8	H	130/180 (72%)	130 (100%)	0	100	100
9	I	104/146 (71%)	104 (100%)	0	100	100
10	J	93/118 (79%)	93 (100%)	0	100	100
11	K	91/113 (80%)	91 (100%)	0	100	100
12	L	158/226 (70%)	158 (100%)	0	100	100
13	M	97/113 (86%)	97 (100%)	0	100	100
14	N	96/115 (84%)	96 (100%)	0	100	100
15	O	174/230 (76%)	174 (100%)	0	100	100
16	P	88/123 (72%)	88 (100%)	0	100	100
17	Q	78/78 (100%)	78 (100%)	0	100	100
18	R	264/318 (83%)	264 (100%)	0	100	100
19	S	116/164 (71%)	116 (100%)	0	100	100
20	T	153/157 (98%)	153 (100%)	0	100	100
21	U	152/174 (87%)	152 (100%)	0	100	100
22	V	325/364 (89%)	324 (100%)	1 (0%)	92	98
23	W	87/158 (55%)	87 (100%)	0	100	100
24	X	311/351 (89%)	309 (99%)	2 (1%)	86	95
25	Y	137/357 (38%)	137 (100%)	0	100	100
26	Z	90/95 (95%)	90 (100%)	0	100	100
27	0	188/190 (99%)	188 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	1	254/291 (87%)	253 (100%)	1 (0%)	91	97
29	2	100/100 (100%)	100 (100%)	0	100	100
30	3	65/166 (39%)	65 (100%)	0	100	100
31	4	529/609 (87%)	528 (100%)	1 (0%)	93	98
32	8	172/247 (70%)	172 (100%)	0	100	100
All	All	5224/6590 (79%)	5218 (100%)	6 (0%)	93	98

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
24	X	394	HIS
28	1	305	ASN
31	4	486	TYR
22	V	226	TYR
7	G	389	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
24	X	385	ASN
25	Y	290	ASN
32	8	118	GLN
31	4	257	HIS
31	4	295	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	951/955 (99%)	118 (12%)	0

5 of 118 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	649	A
1	A	651	A
1	A	680	U
1	A	688	A
1	A	704	U

There are no RNA pucker outliers to report.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

8 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
1	MA6	A	1583	1	19,26,27	0.77	0	18,38,41	0.60	0
9	5F0	I	184	9	8,8,9	0.60	0	7,9,11	1.10	1 (14%)
17	AYA	Q	2	17	6,7,8	0.76	0	5,8,10	0.52	0
1	B8T	A	1486	1	16,22,23	0.72	0	17,31,34	0.44	0
1	5MC	A	1488	1	15,22,23	0.77	1 (6%)	19,32,35	1.10	2 (10%)
29	AYA	2	2	29	6,7,8	0.79	0	5,8,10	0.57	0
1	MA6	A	1584	1	19,26,27	0.78	0	18,38,41	0.56	0
1	5MU	A	1076	1	15,22,23	1.10	1 (6%)	16,32,35	3.66	2 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MA6	A	1583	1	-	0/7/29/30	0/3/3/3
9	5F0	I	184	9	-	0/9/9/10	-
17	AYA	Q	2	17	-	0/4/6/8	-
1	B8T	A	1486	1	-	0/7/27/28	0/2/2/2
1	5MC	A	1488	1	-	0/5/25/26	0/2/2/2
29	AYA	2	2	29	-	0/4/6/8	-
1	MA6	A	1584	1	-	2/7/29/30	0/3/3/3
1	5MU	A	1076	1	-	0/5/25/26	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1076	5MU	C4-N3	3.12	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1488	5MC	C6-C5	-2.07	1.34	1.40

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1076	5MU	C2-N3-C4	14.25	127.18	115.14
1	A	1488	5MC	C4-N3-C2	3.57	120.33	116.02
9	I	184	5F0	OD1-C1-CB	-2.37	118.53	125.43
1	A	1488	5MC	CM5-C5-C6	2.15	123.22	118.68
1	A	1076	5MU	C5M-C5-C6	2.07	123.06	118.68

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1584	MA6	C5-C6-N6-C9
1	A	1584	MA6	C4'-C5'-O5'-P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1584	MA6	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 96 ligands modelled in this entry, 92 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
37	ATP	X	501	33	26,33,33	0.76	0	31,52,52	0.63	0
36	FES	T	201	20,13	0,4,4	-	-	-		
36	FES	P	201	5,16	0,4,4	-	-	-		
38	GDP	X	502	-	24,30,30	0.94	1 (4%)	31,47,47	2.10	5 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	ATP	X	501	33	-	0/18/38/38	0/3/3/3
36	FES	T	201	20,13	-	-	0/1/1/1
36	FES	P	201	5,16	-	-	0/1/1/1
38	GDP	X	502	-	-	0/12/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	X	502	GDP	C6-N1	3.07	1.38	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	X	502	GDP	C5-C6-N1	-8.41	111.92	123.43
38	X	502	GDP	C2-N1-C6	5.98	125.43	115.93
38	X	502	GDP	N3-C2-N1	-2.87	123.40	127.22
38	X	502	GDP	C2-N3-C4	-2.54	112.45	115.36
38	X	502	GDP	C4-C5-C6	-2.47	118.44	120.80

There are no chirality outliers.

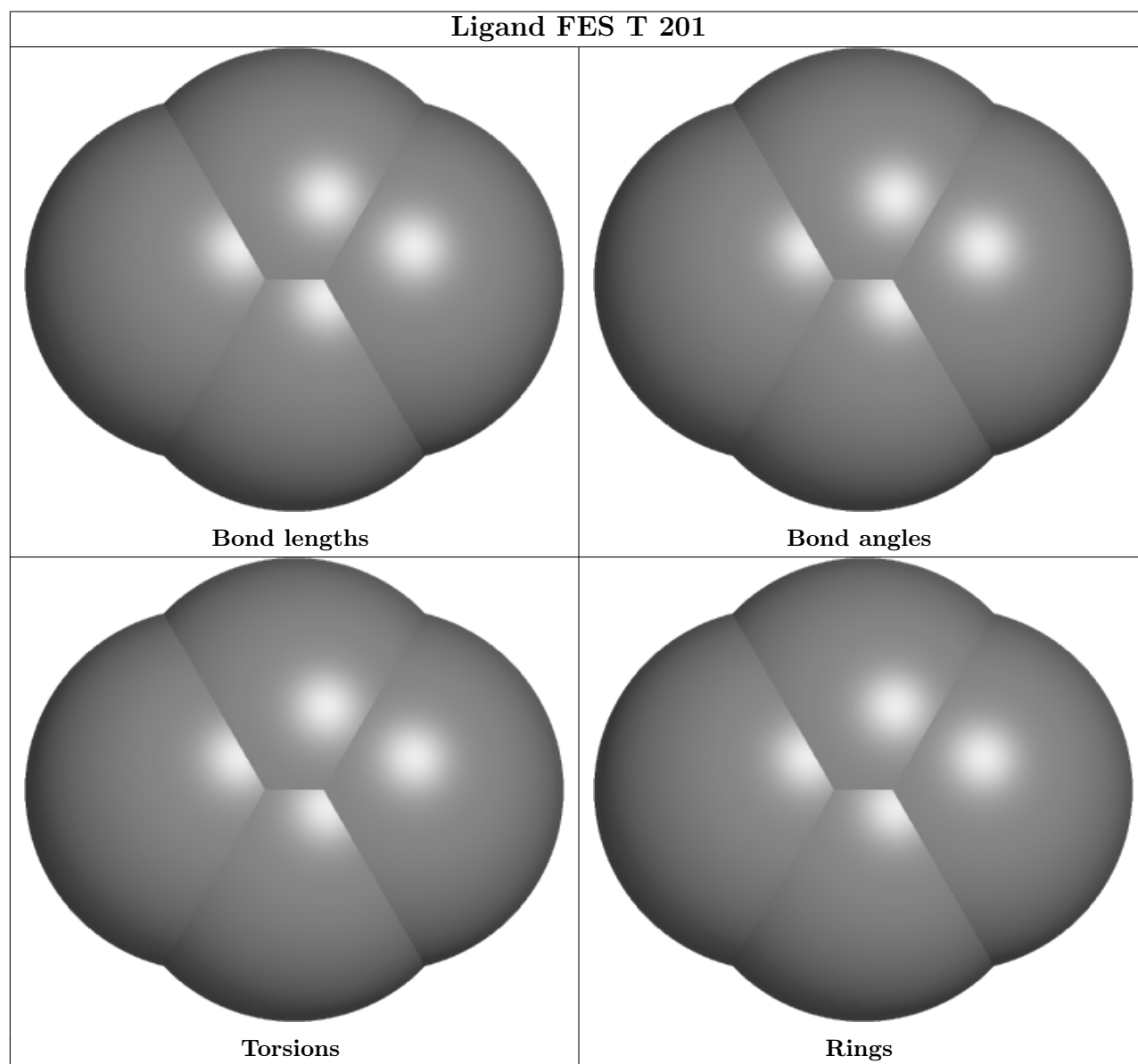
There are no torsion outliers.

There are no ring outliers.

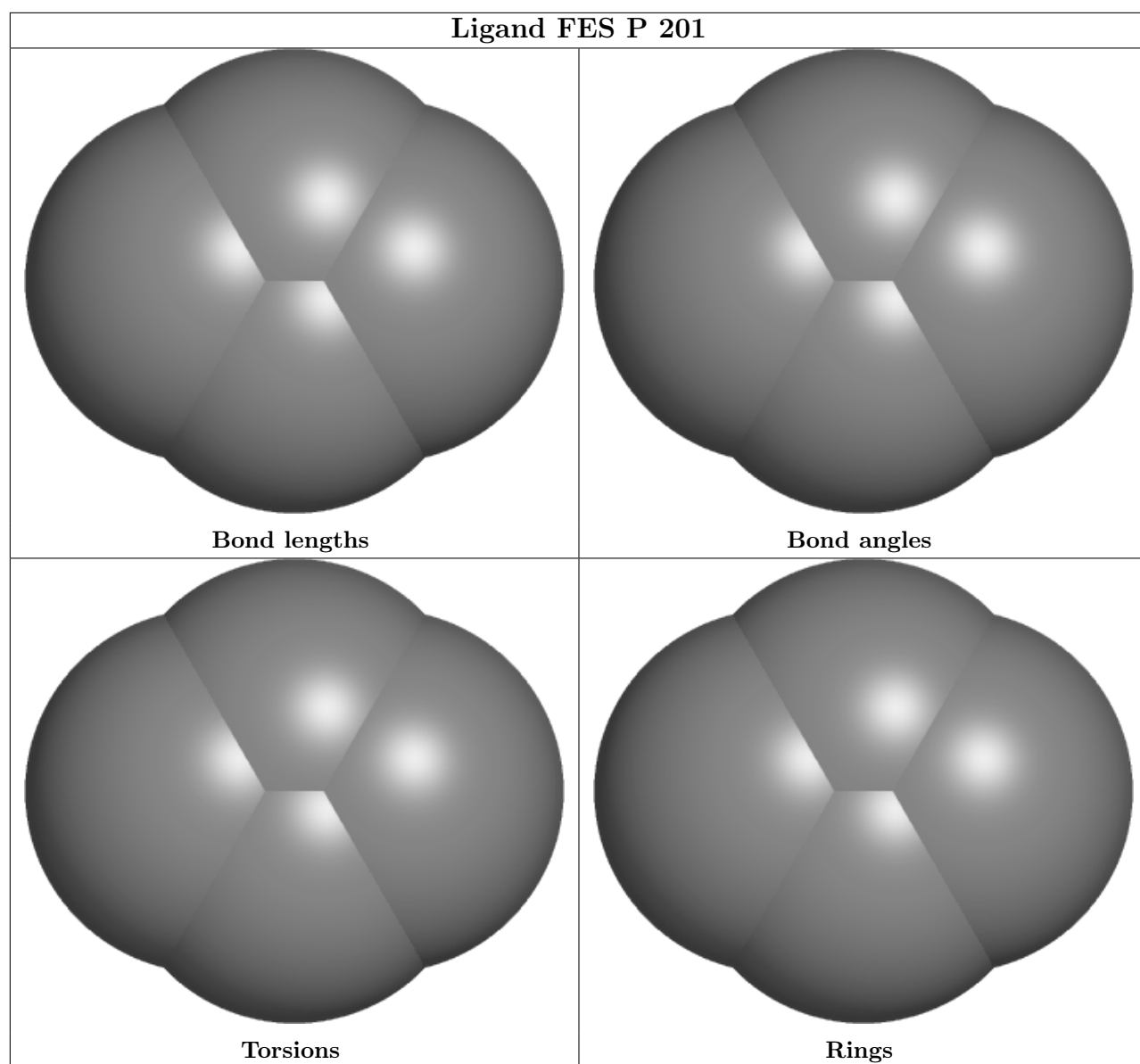
No monomer is involved in short contacts.

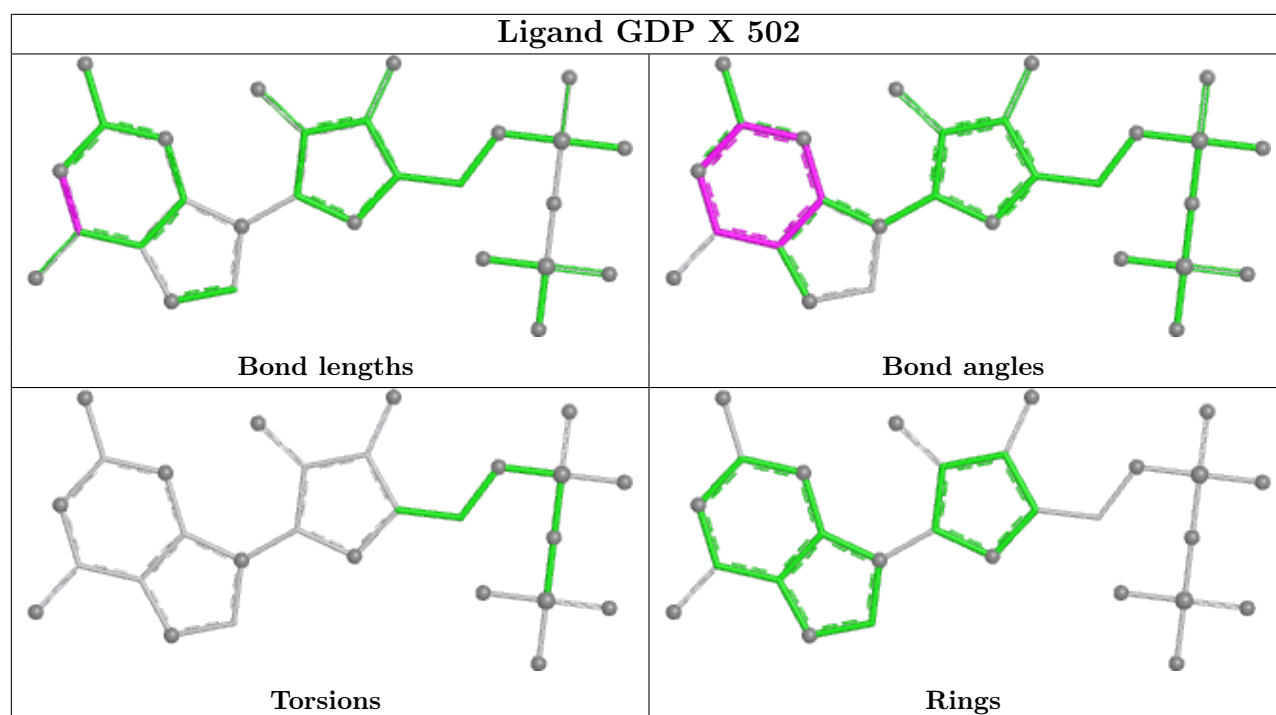
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

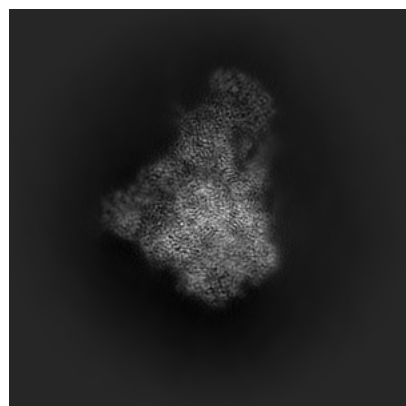
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13559. These allow visual inspection of the internal detail of the map and identification of artifacts.

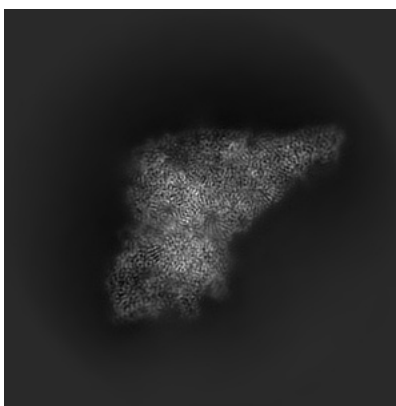
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

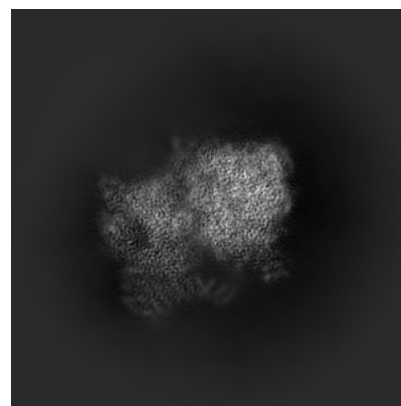
#### 6.1.1 Primary map



X

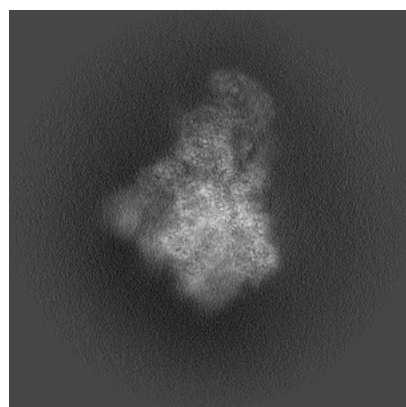


Y

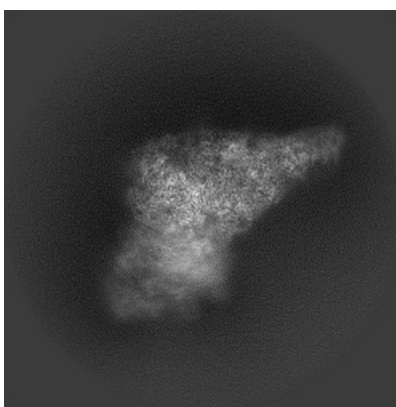


Z

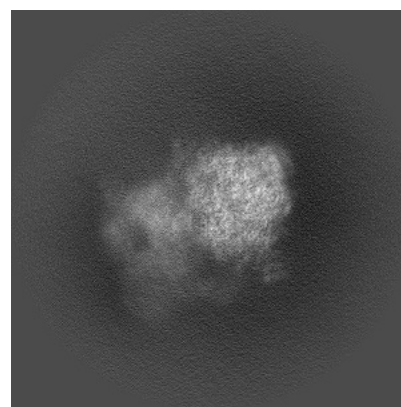
#### 6.1.2 Raw map



X



Y

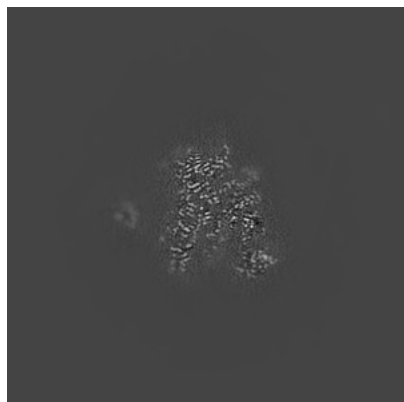


Z

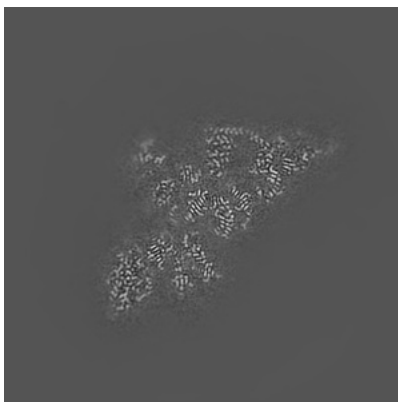
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

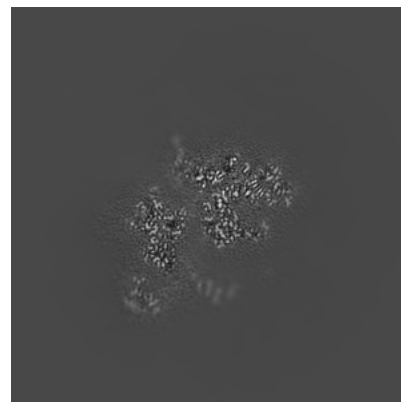
### 6.2.1 Primary map



X Index: 300

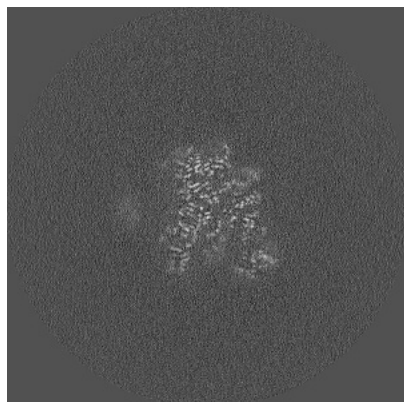


Y Index: 300

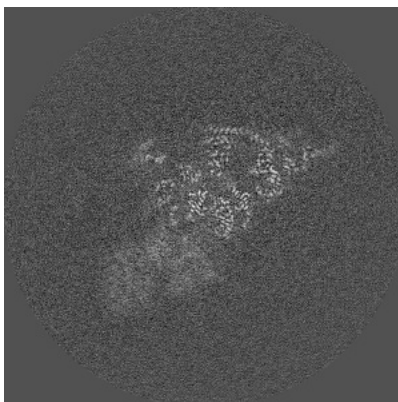


Z Index: 300

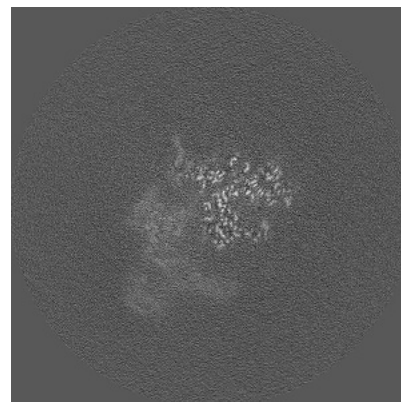
### 6.2.2 Raw map



X Index: 240



Y Index: 240

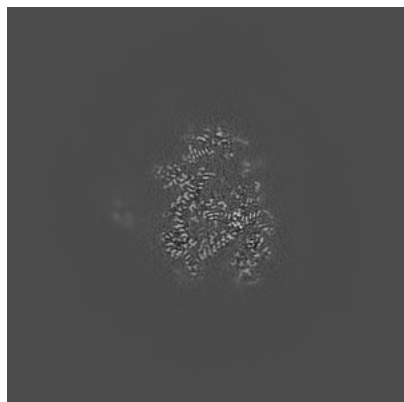


Z Index: 240

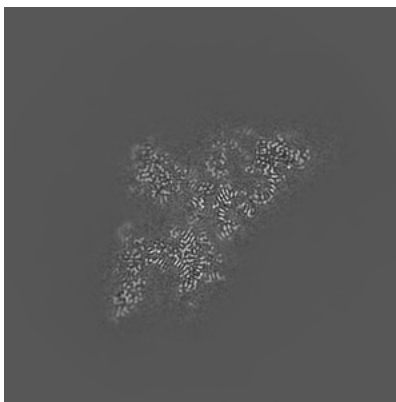
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

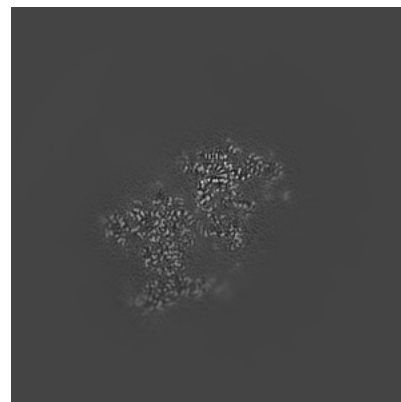
### 6.3.1 Primary map



X Index: 323

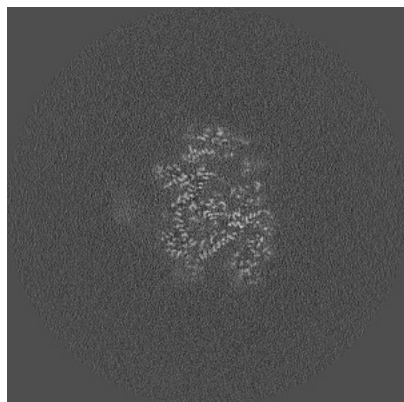


Y Index: 291

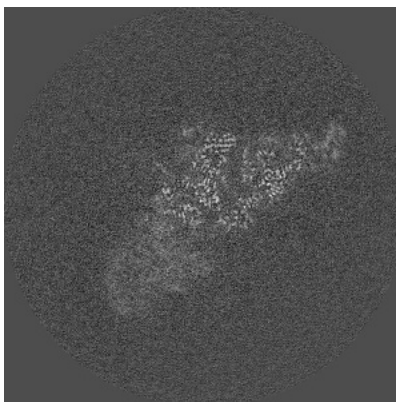


Z Index: 276

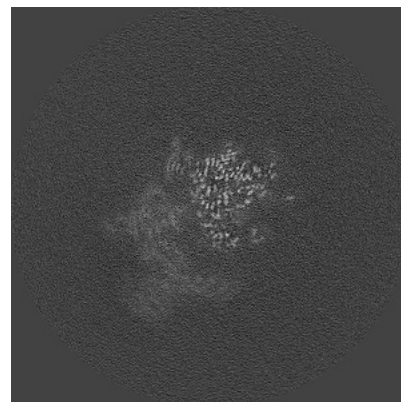
### 6.3.2 Raw map



X Index: 258



Y Index: 254

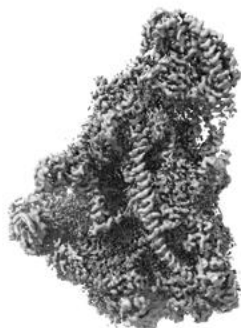


Z Index: 231

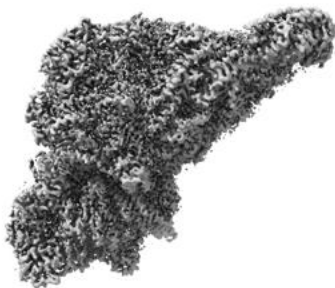
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



X



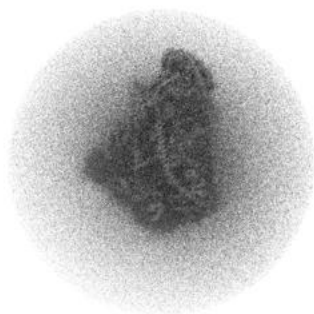
Y



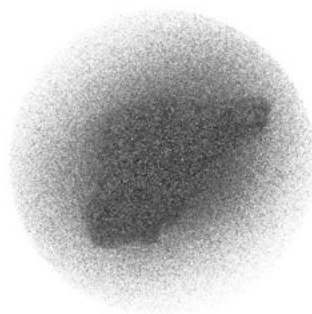
Z

The images above show the 3D surface view of the map at the recommended contour level 0.12. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

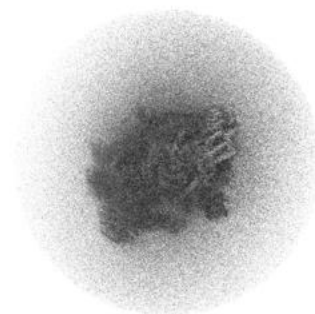
### 6.4.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

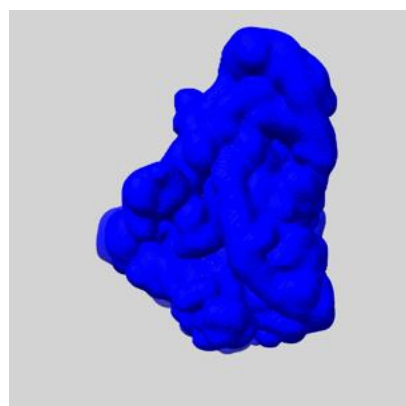
## 6.5 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

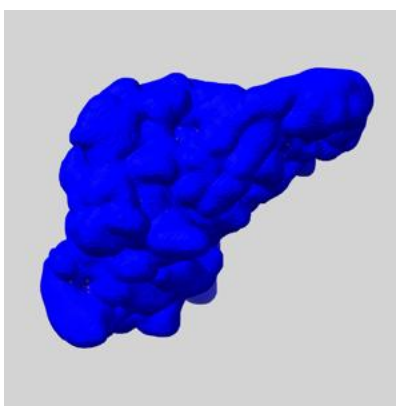
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

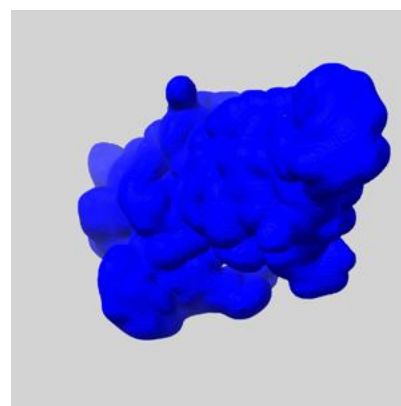
### 6.5.1 emd\_13559\_msk\_1.map [i](#)



X



Y



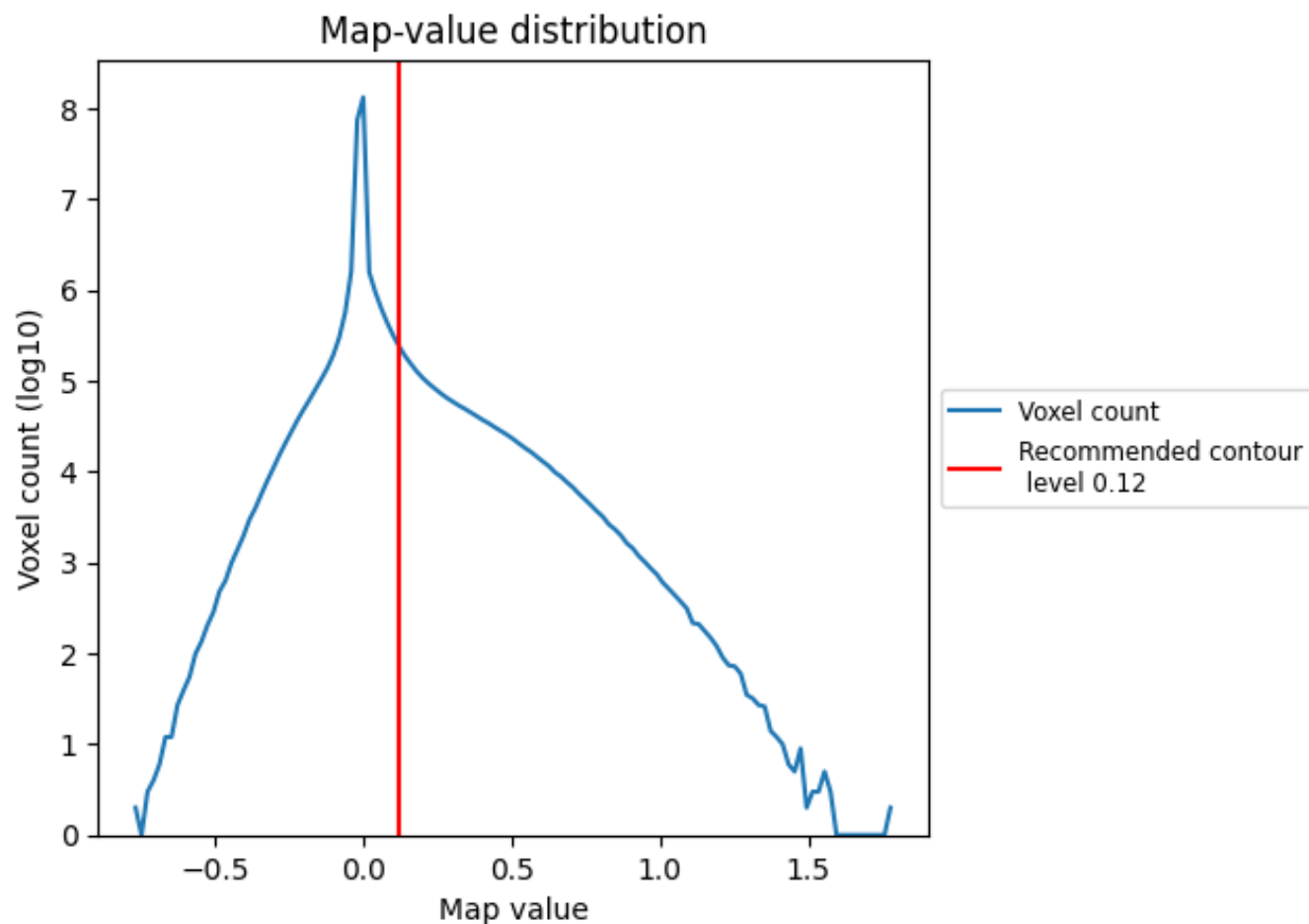
Z



## 7 Map analysis [i](#)

This section contains the results of statistical analysis of the map.

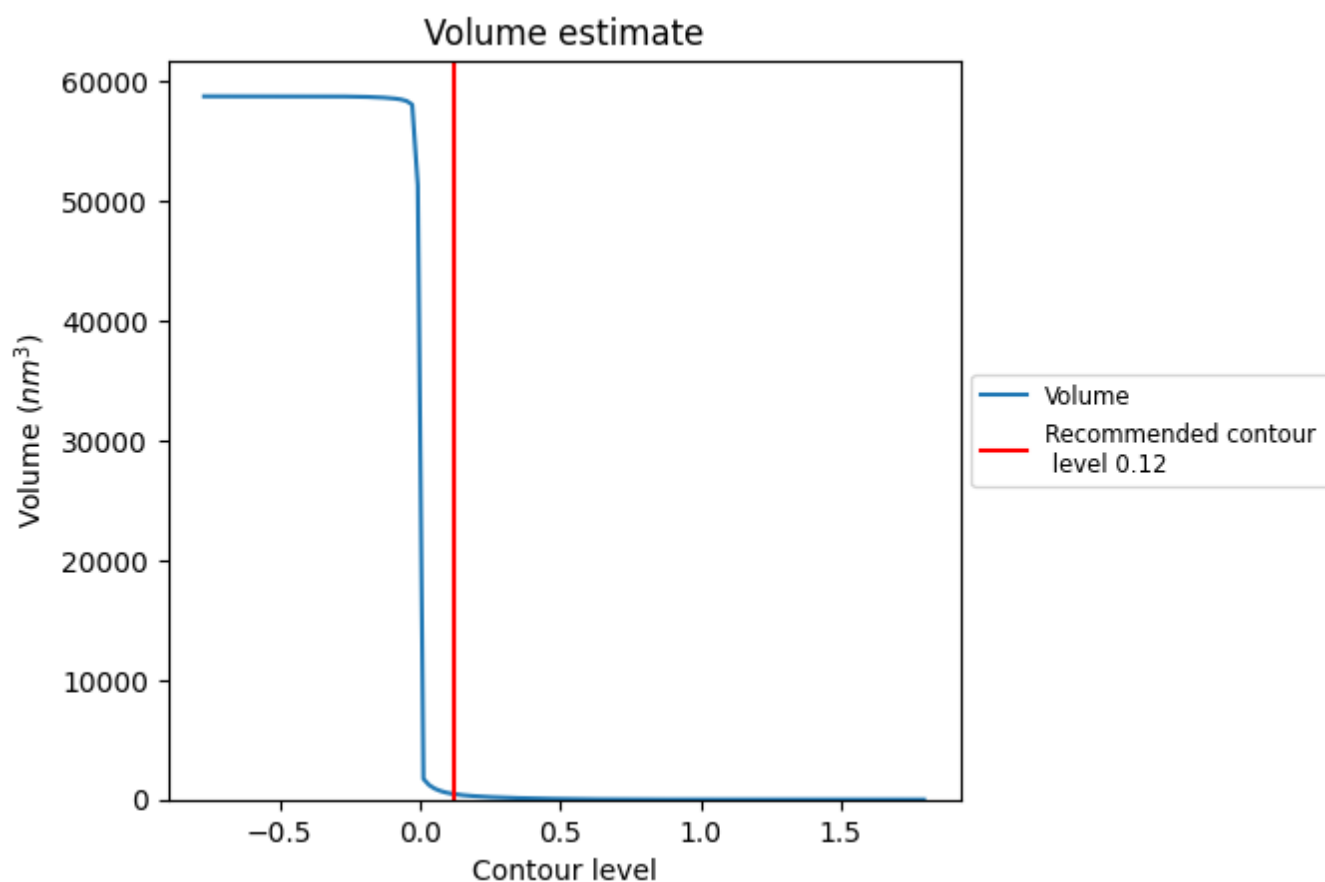
### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.



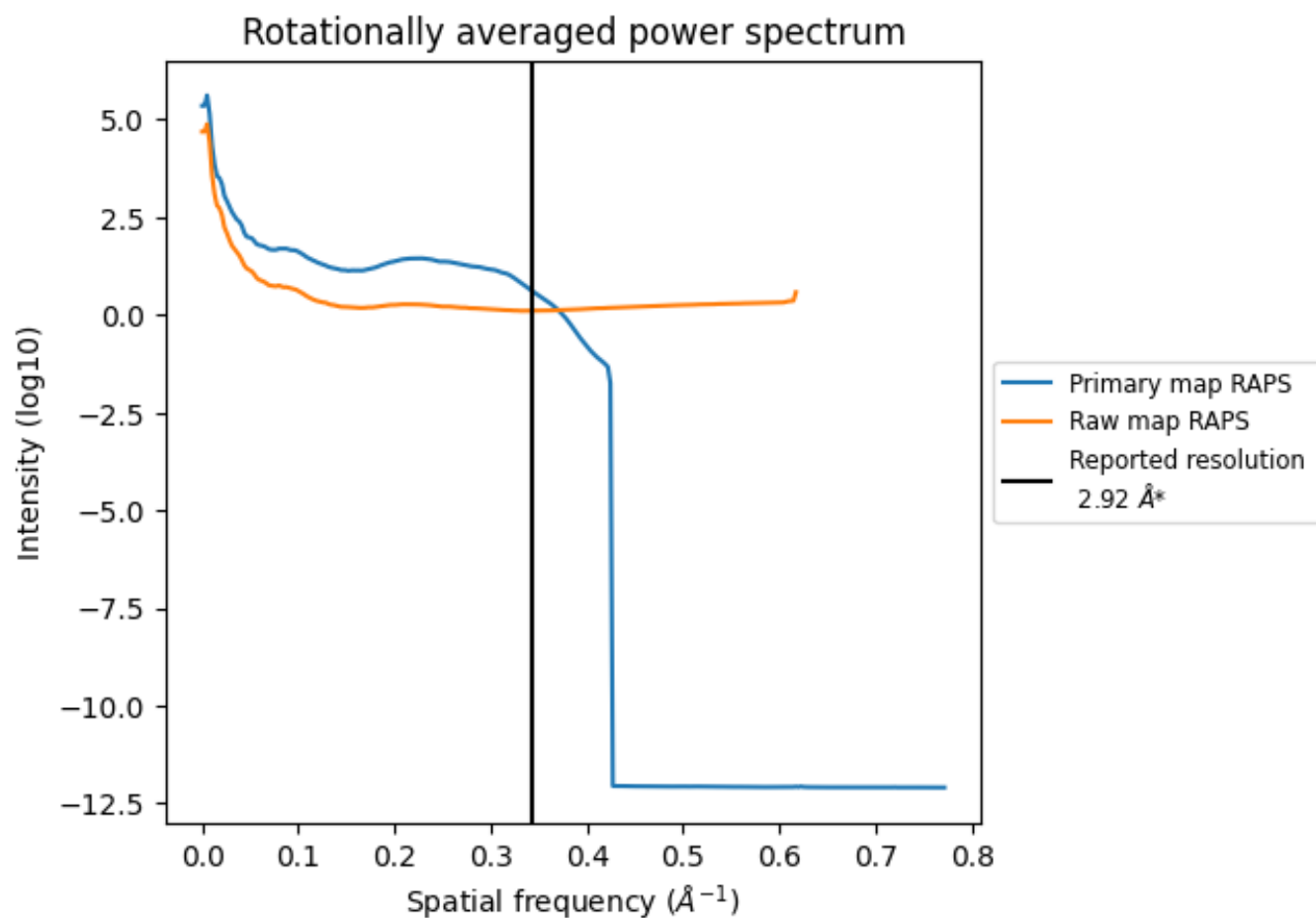
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 465  $\text{nm}^3$ ; this corresponds to an approximate mass of 420 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ

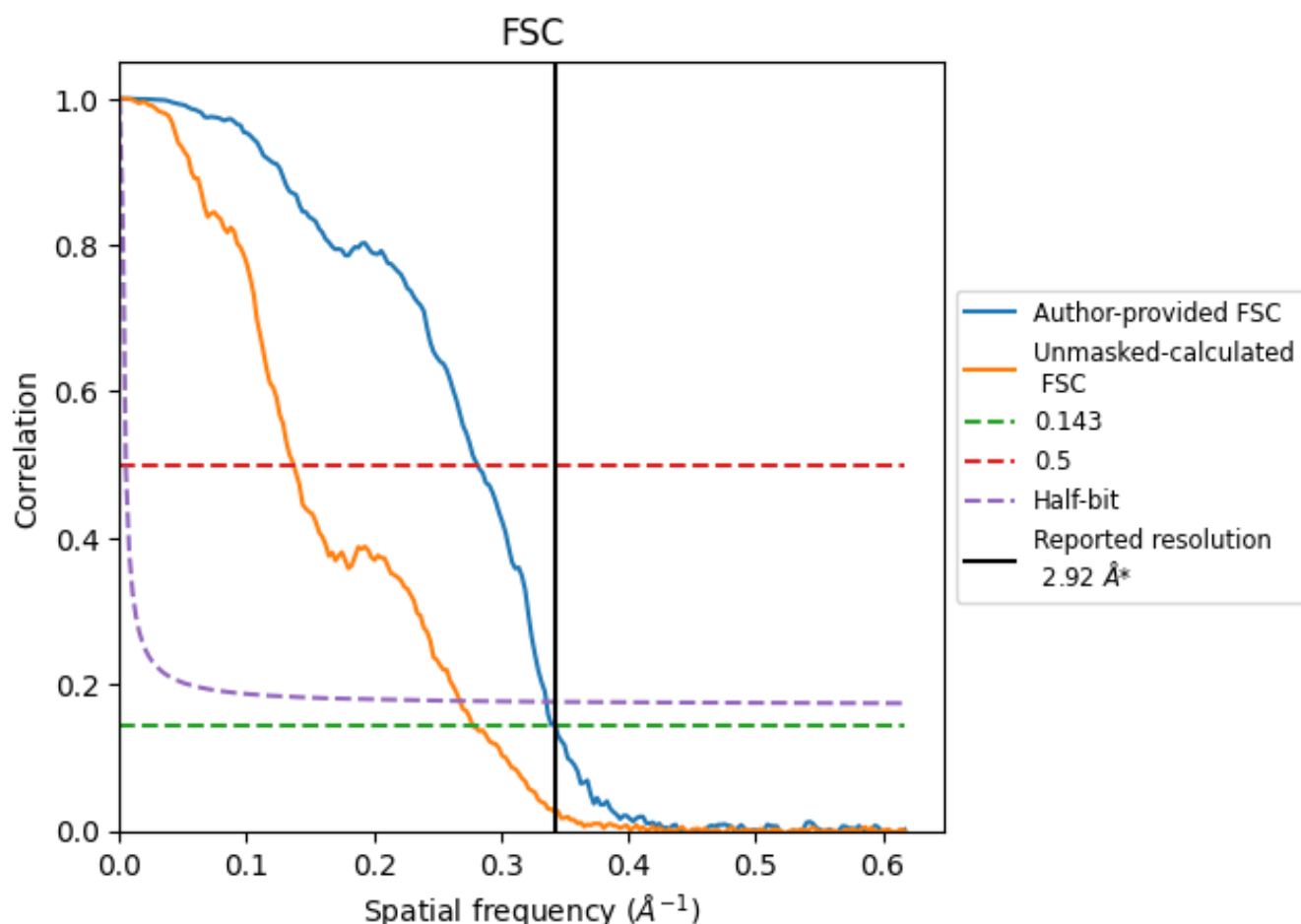


\*Reported resolution corresponds to spatial frequency of 0.342 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.342 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

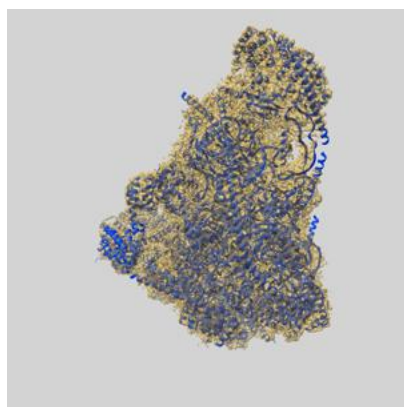
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.92	-	-
Author-provided FSC curve	2.92	3.56	2.98
Unmasked-calculated*	3.60	7.31	3.74

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.60 differs from the reported value 2.92 by more than 10 %

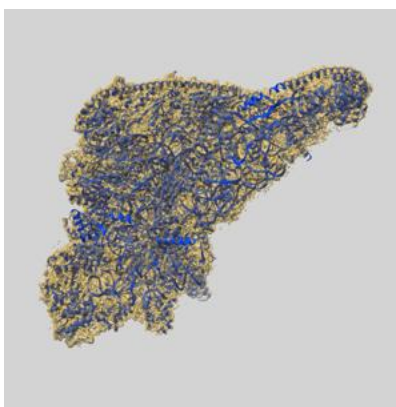
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-13559 and PDB model 7PO1. Per-residue inclusion information can be found in section [3](#) on page [13](#).

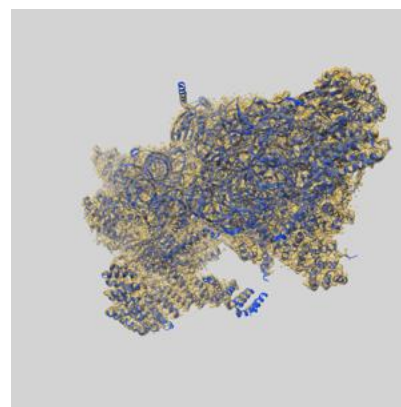
### 9.1 Map-model overlay [i](#)



X



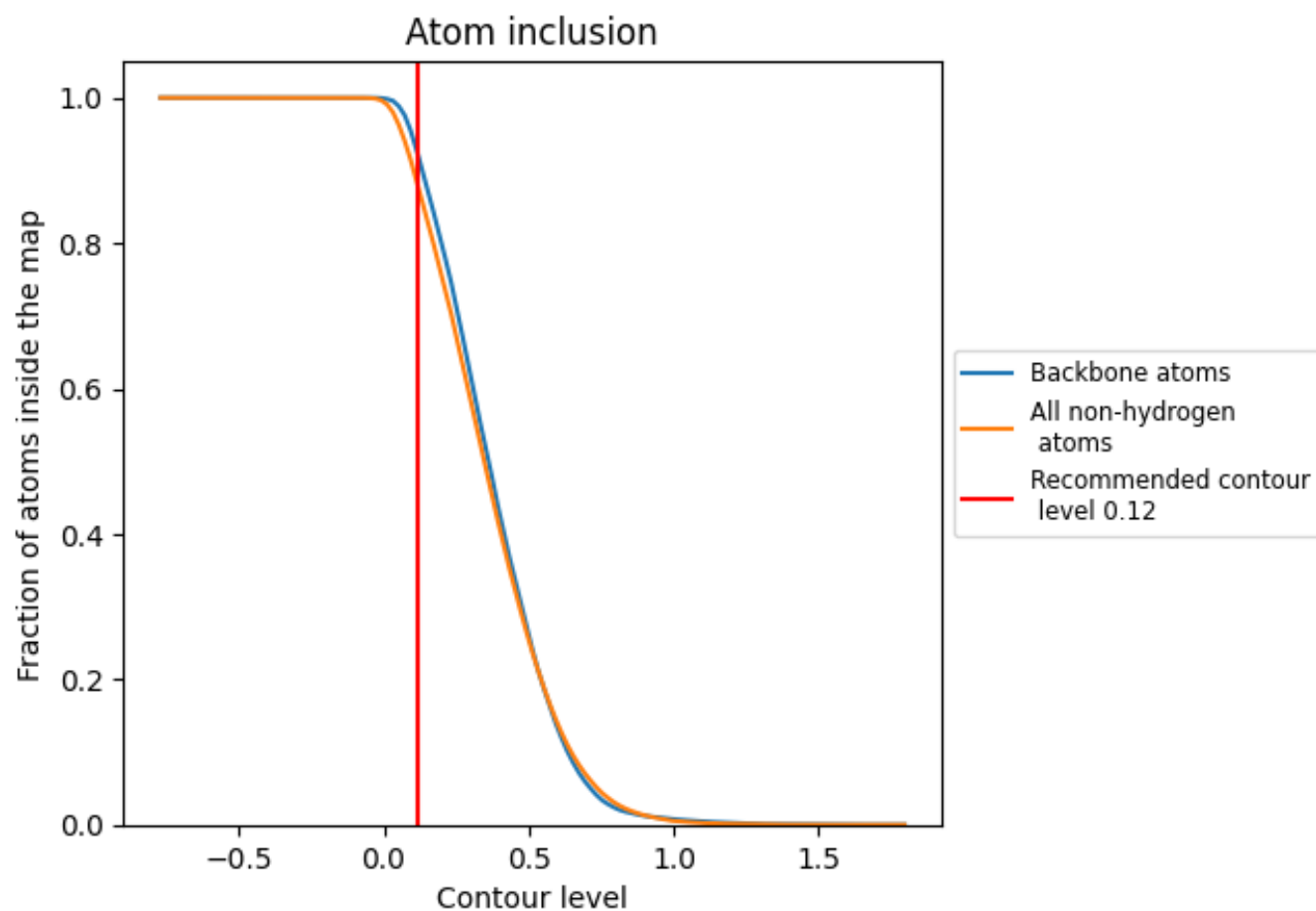
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.